Connecting via Winsock to STN

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* * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:21:34 ON 22 JUL 2009

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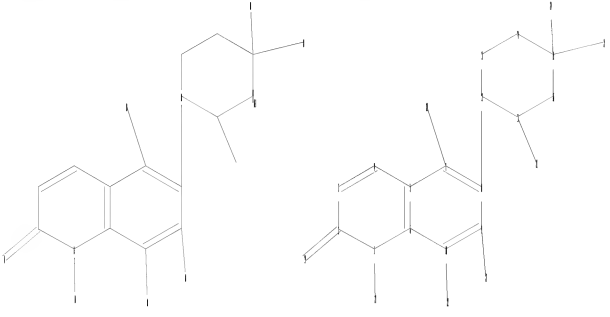
Uploading C:\Program Files\Stnexp\Queries\10566569.str

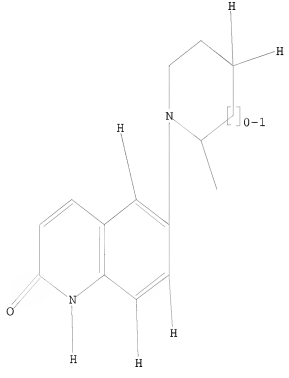


chain nodes :
19 20 21 22 23 24 25 27
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
1-27 2-19 7-20 8-12 9-21 10-22 11-23 15-24 15-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16
exact/norm bonds :
1-2 1-6 2-3 2-19 3-4 4-5 8-12 11-12 11-16 12-13 13-14 14-15 15-16
exact bonds :
1-27 7-20 9-21 10-22 11-23 15-24 15-25
normalized bonds :
5-6 5-7 6-10 7-8 8-9 9-10
isolated ring systems :
containing 1 : 11 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam
SAMPLE SEARCH INITIATED 13:22:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 510 TO ITERATE

100.0% PROCESSED 510 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

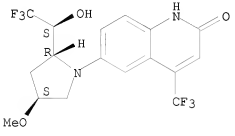
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8846 TO 11554
PROJECTED ANSWERS: 9 TO 360

```
L2            9 SEA SSS SAM L1

=> d scan

L2   9 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   2(1H)-Quinolinone, 6-[(2R,4S)-4-methoxy-2-[(1S)-2,2,2-trifluoro-1-
     hydroxyethyl]-1-pyrrolidinyl]-4-(trifluoromethyl)-
MF   C17 H16 F6 N2 O3

Absolute stereochemistry.
```

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l1 full
FULL SEARCH INITIATED 13:22:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    10692 TO ITERATE

100.0% PROCESSED    10692 ITERATIONS                          192 ANSWERS
SEARCH TIME: 00.00.01

L3          192 SEA SSS FUL L1

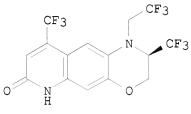
=> file ca


=> s l3
L4            5 L3

=> d ibib abs fhitstr 1-5

L4   ANSWER 1 OF 5  CA  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         149:118675  CA
TITLE:                    Selective androgen receptor modulators based on a
                          series of 7H-[1,4]oxazino[3,2-g]quinolin-7-ones with
                          improved in vivo activity
AUTHOR(S):                Long, Yun Oliver; Higuchi, Robert I.; Caferro, Thomas
                          R.; Lau, Thomas L. S.; Wu, Min; Cummings, Marquis L.;
                          Martinborough, Esther A.; Marschke, Keith B.; Chang,
                          William Y.; Lopez, Francisco J.; Karanewsky, Donald
                          S.; Zhi, Lin
CORPORATE SOURCE:         Discovery Research, Ligand Pharmaceuticals, San Diego,
```

CA, 92121, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(9), 2967-2971
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:118675
GI



I

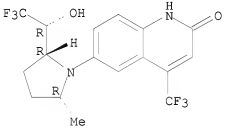
AB Modification on a lead series of [1,4]oxazino[3,2-g]quinolin-7-ones at the 2-position led to selective androgen receptor modulators with improved in vivo activity. The most potent analog (-)-33a(I) exhibited full maintenance of levator ani muscle at 3 mg/kg and reduced activity on ventral prostate weight in a 2-wk orally-dosed and orchidectomized rat maintenance assay.

IT 847235-85-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Selective androgen receptor modulators based on a series of 7H-[1,4]oxazino[3,2-g]quinolin-7-ones with improved in vivo activity)

RN 847235-85-2 CA

CN 2(1H)-Quinolinone, 6-[(2R,5R)-2-methyl-5-[(1R)-2,2,2-trifluoro-1-hydroxyethyl]-1-pyrrolidinyl]-4-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

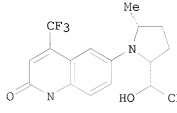
L4 ANSWER 2 OF 5 CA COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:534026 CA

TITLE: Substituted 6-(1-Pyrrolidine)quinolin-2(1H)-ones as Novel Selective Androgen Receptor Modulators

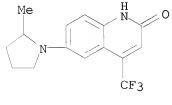
AUTHOR(S): Martinborough, Esther; Shen, Yixing; Van Oeveren,

Arjan; Long, Yun Oliver; Lau, Thomas L. S.; Marschke, Keith B.; Chang, William Y.; Lopez, Francisco J.; Vajda, Eric G.; Rix, Peter J.; Viveros, O. Humberto; Negro-Vilar, Andres; Zhi, Lin
CORPORATE SOURCE: Discovery Research, Ligand Pharmaceuticals Inc., San Diego, CA, 92121, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(21), 5049-5052
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:534026
GI



I

AB The androgen receptor is a ligand inducible transcription factor that is involved in a broad range of physiol. functions. Here we describe the discovery of a new class of orally available selective androgen receptor modulators. The lead compound, 6-[(2R,5R)-2-methyl-5-((R)-2,2,2-trifluoro-1-hydroxyethyl)pyrrolidin-1-yl]-4-trifluoromethylquinolin-2(1H)-one (6a)(I), showed excellent anabolic activity in muscle with reduced effect on the prostate in a rat model of hypogonadism. The compound also improved bone strength in a rat model of post-menopausal osteoporosis.
IT 328949-90-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Substituted 6-(1-Pyrrolidine)quinolin-2(1H)-ones as Novel Selective Androgen Receptor Modulators)
RN 328949-90-2 CA
CN 2(1H)-Quinolinone, 6-(2-methyl-1-pyrrolidinyl)-4-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 146:142515 CA
TITLE: Quinolinones, chromenones, benzothiopyranones, and anilines as androgen receptor modulators, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Loren, Jon C.; Miller, Todd; Pedram, Bijan; Rowley, Charlene V.; Shen, Yixing; Van Oeveren, Cornelis A.; Zhi, Lin
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007005887	A2	20070111	WO 2006-US26067	20060630
WO 2007005887	A3	20070419		

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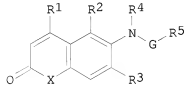
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-695949P P 20050701
OTHER SOURCE(S): CASREACT 146:142515; MARPAT 146:142515
GI



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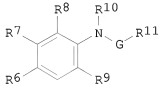
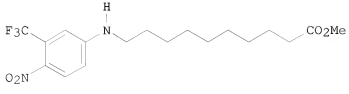


II



III

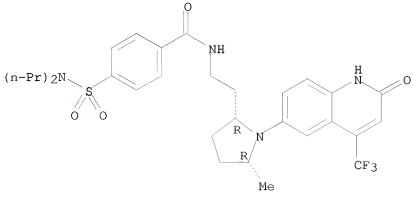
AB The invention relates to compds. of general formulas I, II or related derivs., which are androgen receptor modulators. In compds. I, X is O, S, or (un)substituted N; G is a bond, C(O), C(S), or S(O)2; R1, R2, and R3 are independently selected from H, halo, OH, SH, NH2, C1-6 alkoxy, C1-6 haloalkoxy, C1-6 alkylthio, C1-6 alkylamino, (un)substituted C1-4 alkyl, (un)substituted C1-4 haloalkyl, etc.; and R4 and R5 are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, etc.; including pharmaceutically acceptable salts and prodrugs thereof. In compds. II, G is as defined previously; R6 and R7 are independently selected from halo, cyano, nitro, C1-4 alkyl, C1-4 haloalkyl, C1-4 heteroalkyl, and C1-4 heterohaloalkyl; R8 and R9 are independently selected from H, halo, OH, SH, NH2, C1-6 alkoxy, C1-6 haloalkoxy, C1-6 alkylthio, C1-6 alkylamino, (un)substituted C1-4 alkyl, (un)substituted C1-4 haloalkyl, (un)substituted C1-4 heteroalkyl, etc.; and R10 and R11 are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, etc.; including pharmaceutically acceptable salts and prodrugs thereof. The invention also relates to the preparation of the compds. of the invention, pharmaceutical compns. comprising a compound of the invention and a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment or prevention of conditions that respond to androgen receptor modulation, such as acne, male-pattern baldness, infertility, and impotence. Substitution of Me 10-bromodecanoate with 4-nitro-3-trifluoromethylaniline gave aminodecanoate III. Some compds. of the invention are agonists of androgen receptors, but other compds. are antagonists of androgen receptors (no data).

IT 918895-56-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of quinolinones, chromenones, benzothiopyranones, and anilines for use as androgen receptor modulators)

RN 918895-56-4 CA

CN Benzamide, N-[2-[(2R,5R)-1-[1,2-dihydro-2-oxo-4-(trifluoromethyl)-6-quinolinyl]-5-methyl-2-pyrrolidinyl]ethyl]-4-[(dipropylamino)sulfonyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 142:280067 CA
TITLE: Preparation of 6-pyrrolidinyl- and 6-piperidinylquinolinones as androgen receptor modulators
INVENTOR(S): Zhi, Lin; Martinborough, Esther; Shen, Yixing; Stevens Lau, Thomas Lot; Wu, Min; Long, Yun Oliver
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005018573	A2	20050303	WO 2004-US27483	20040823
WO 2005018573	A3	20050506		
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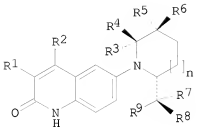
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004266160	A1	20050303	AU 2004-266160	20040823
CA 2536349	A1	20050303	CA 2004-2536349	20040823
EP 1656142	A2	20060517	EP 2004-782052	20040823
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1838956	A	20060927	CN 2004-80024125	20040823
BR 2004013820	A	20061024	BR 2004-13820	20040823
JP 2007503398	T	20070222	JP 2006-524121	20040823
MX 2006001751	A	20060512	MX 2006-1751	20060214
IN 2006MN00272	A	20070608	IN 2006-MN272	20060308
US 20070066650	A1	20070322	US 2006-566569	20060821
US 20080227810	A9	20080918		
IN 2009MN00090	A	20090515	IN 2009-MN90	20090109

PRIORITY APPLN. INFO.:			
	US 2003-497125P	P	20030822
	WO 2004-US27483	W	20040823
	IN 2006-MN272	A3	20060308

OTHER SOURCE(S): MARPAT 142:280067
GI



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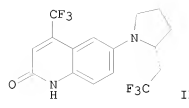


II

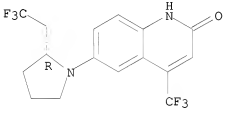
AB Title compds. I [wherein R1 = H, F, Cl or alkyl; R2 = H, halo, (un)substituted alkyl; R3, R4 = H, (un)substituted alkyl or (hetero)aryl; R5, R6 = OH, OPh, OBn or alkoxy; R5 - R8 = H, F, Cl or (un)substituted alkyl; R7 and R8 taken together form a CO; R9 = H, thioether, (un)substituted amine, alkyl, etc.; n = 0-1; and pharmaceutically acceptable salts thereof], e.g., II, were prepared as androgen receptor (AP) modulators. Biol. assays were performed, but no data were reported. Also disclosed are pharmaceutical compns. of I, methods for modulating processes mediated by AR, and their medical uses in the treatment of such as acne and sexual dysfunction.

IT 847235-72-7P, (R)-6-[2-(2,2,2-Trifluoroethyl)-1-pyrrolidinyl]-4-trifluoromethyl-2(1H)-quinolinone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(modulator; preparation of pyrrolidinyl- and piperidinylquinolinones as androgen receptor modulators)

RN 847235-72-7 CA

CN 2(1H)-Quinolinone, 6-[(2R)-2-(2,2,2-trifluoroethyl)-1-pyrrolidinyl]-4-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 5 CA COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:207727 CA

TITLE: Preparation of quinolinones and related bicyclic compounds as androgen and progesterone receptor modulators.

INVENTOR(S): Zhi, Lin; Tegley, Christopher; Pio, Barbara; Arjan van Oeveren, Cornelis; Motamedi, Mehrnouch; Martinborough, Esther; West, Sarah; Higuchi, Robert; Hamann,

Lawrence; Farmer, Luc
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 356 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016108	A2	20010308	WO 2000-US23585	20000825
WO 2001016108	A3	20011220		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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US 6566372	B1	20030520	US 2000-649466	20000824
CA 2384435	A1	20010308	CA 2000-2384435	20000825
BR 2000013653	A	20020514	BR 2000-13653	20000825
EP 1212303	A2	20020612	EP 2000-959507	20000825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200508	T2	20020923	TR 2002-508	20000825
CN 1382124	A	20021127	CN 2000-814750	20000825
CN 1262540	C	20060705		
JP 2003508387	T	20030304	JP 2001-519677	20000825
HU 2002004337	A2	20030328	HU 2002-4337	20000825
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AU 782647	B2	20050818	AU 2000-70819	20000825
CN 1775759	A	20060524	CN 2005-10112855	20000825
CN 100384823	C	20080430		
CN 101029042	A	20070905	CN 2006-10078531	20000825
ZA 2002001053	A	20030528	ZA 2002-1053	20020206
IN 2002MN00201	A	20051104	IN 2002-MN201	20020215
NO 2002000912	A	20020429	NO 2002-912	20020225
MX 2002002027	A	20030519	MX 2002-2027	20020226
BG 106539	A	20021031	BG 2002-106539	20020321
US 20030130505	A1	20030710	US 2002-299909	20021118
US 6964973	B2	20051115		
US 20050288350	A1	20051229	US 2005-165769	20050623

PRIORITY APPLN. INFO.:
US 1999-150987P P 19990827
US 2000-649466 A3 20000824
CN 2000-814750 A3 20000825
WO 2000-US23585 W 20000825
US 2002-299909 A3 20021118

OTHER SOURCE(S): MARPAT 134:207727
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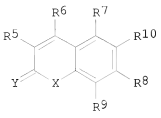


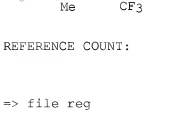
I

AB Title compds., e.g. [I; R1, R2 = COR3, CSR3, SO2R3, NO, NR3R4, alkyl, alkenyl, haloalkyl, haloalkenyl, haloalkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, etc.; R1R2 = atoms to form (substituted) heterocyclyl; R3, R4 = H, (substituted) alkyl, alkenyl, alkynyl, haloalkyl, heteroalkyl, heteroaryl, aryl; R5 = H, F, Cl, Br, iodo, OR3, SR3, NR3R4, alkyl, haloalkyl, heteroalkyl; R6 = F, Cl, Br, iodo, Me, CF3, CHF2, cyano, CF2Cl, CF2OR3, OR3, SOR3, CO2R3, NR3R4, (substituted) alkyl, alkenyl, alkynyl, haloalkyl, heteroalkyl, etc.; R7, R8 = H, F, Cl, Br, iodo, cyano, OR3, NR3R4, SR3, SOR3, NR3COR4, alkyl, haloalkyl, heteroalkyl, etc.; R9 = H, F, Cl, iodo, OR3, NR3R4, SR3, SOR3, SO2R3, alkyl, haloalkyl, heteroalkyl; R10 = NR1R2, (substituted) heterocyclyl; Y = O, S, NR3, NOR3, CR3R4], were prepared Thus, 6-amino-4-trifluoromethyl-2(1H)-quinolinone (preparation given) was stirred with propionaldehyde and NaBH3CN in MeOH to give 70-95% 6-propylamino-4-trifluoromethyl-2(1H)-quinolinone. The latter showed androgen receptor agonist activity with a potency of 27 nM. A drug composition is given. [This abstract record is one of 2 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 328949-67-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

RN 328949-67-3 CA

CN 2(1H)-Quinolinone, 6-(2-methyl-1-piperidinyl)-4-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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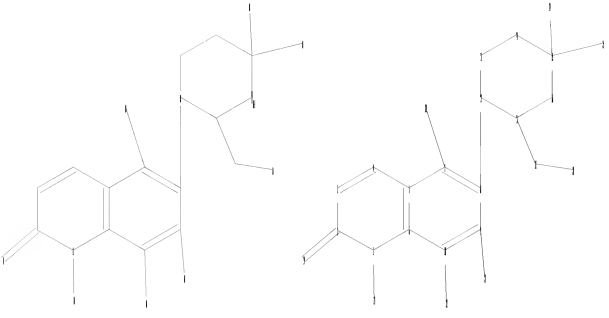

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19 20 21 22 23 24 25 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
1-27 2-19 7-20 8-12 9-21 10-22 11-23 15-24 15-25 23-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16
exact/norm bonds :
1-2 1-6 2-3 2-19 3-4 4-5 8-12 11-12 11-16 12-13 13-14 14-15 15-16
23-28
exact bonds :
1-27 7-20 9-21 10-22 11-23 15-24 15-25
normalized bonds :
5-6 5-7 6-10 7-8 8-9 9-10
isolated ring systems :
containing 1 : 11 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS

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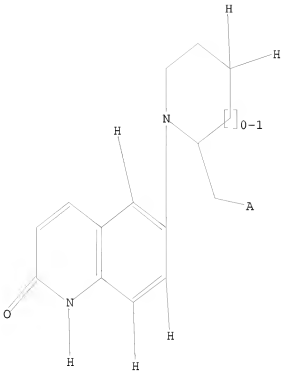

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L6 173 SEA SSS FUL L5

=> file ca

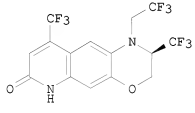
This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family of databases will soon be updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 22.

=> s l6
L7 5 L6

=> d ibib abs fhitstr 1-5

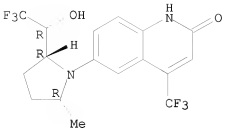
L7 ANSWER 1 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 149:118675 CA
TITLE: Selective androgen receptor modulators based on a series of 7H-[1,4]oxazino[3,2-g]quinolin-7-ones with improved in vivo activity
AUTHOR(S): Long, Yun Oliver; Higuchi, Robert I.; Caferro, Thomas R.; Lau, Thomas L. S.; Wu, Min; Cummings, Marquis L.; Martinborough, Esther A.; Marschke, Keith B.; Chang, William Y.; Lopez, Francisco J.; Karanewsky, Donald S.; Zhi, Lin
CORPORATE SOURCE: Discovery Research, Ligand Pharmaceuticals, San Diego, CA, 92121, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(9), 2967-2971
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:118675
GI



I

AB Modification on a lead series of [1,4]oxazino[3,2-g]quinolin-7-ones at the 2-position led to selective androgen receptor modulators with improved in vivo activity. The most potent analog (-)-33a(I) exhibited full maintenance of levator ani muscle at 3 mg/kg and reduced activity on ventral prostate weight in a 2-wk orally-dosed and orchidectomized rat maintenance assay.
IT 847235-85-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Selective androgen receptor modulators based on a series of 7H-[1,4]oxazino[3,2-g]quinolin-7-ones with improved in vivo activity)
RN 847235-85-2 CA
CN 2(1H)-Quinolinone, 6-[(2R,5R)-2-methyl-5-[(1R)-2,2,2-trifluoro-1-hydroxyethyl]-1-pyrrolidinyl]-4-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 147:534026 CA
TITLE: Substituted 6-(1-Pyrrolidine)quinolin-2(1H)-ones as Novel Selective Androgen Receptor Modulators
AUTHOR(S): Martinborough, Esther; Shen, Yixing; Van Oeveren, Arjan; Long, Yun Oliver; Lau, Thomas L. S.; Marschke, Keith B.; Chang, William Y.; Lopez, Francisco J.; Vajda, Eric G.; Rix, Peter J.; Viveros, O. Humberto; Negro-Vilar, Andres; Zhi, Lin
CORPORATE SOURCE: Discovery Research, Ligand Pharmaceuticals Inc., San Diego, CA, 92121, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(21), 5049-5052
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:534026
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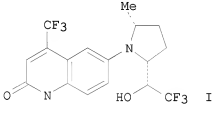
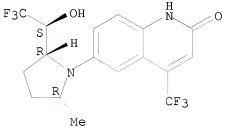


AB The androgen receptor is a ligand inducible transcription factor that is involved in a broad range of physiol. functions. Here we describe the discovery of a new class of orally available selective androgen receptor modulators. The lead compound, 6-[(2R,5R)-2-methyl-5-((R)-2,2,2-trifluoro-1-hydroxyethyl)pyrrolidin-1-yl]-4-trifluoromethylquinolin-2(1H)-one (6a)(I), showed excellent anabolic activity in muscle with reduced effect on the prostate in a rat model of hypogonadism. The compound also improved bone strength in a rat model of post-menopausal osteoporosis.

IT 847235-84-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Substituted 6-(1-Pyrrolidine)quinolin-2(1H)-ones as Novel Selective Androgen Receptor Modulators)
RN 847235-84-1 CA
CN 2(1H)-Quinolinone, 6-[(2R,5R)-2-methyl-5-[(1S)-2,2,2-trifluoro-1-hydroxyethyl]-1-pyrrolidinyl]-4-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 146:142515 CA
TITLE: Quinolinones, chromenones, benzothiopyranones, and anilines as androgen receptor modulators, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Loren, Jon C.; Miller, Todd; Pedram, Bijan; Rowley, Charlene V.; Shen, Yixing; Van Oeveren, Cornelis A.; Zhi, Lin
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007005887	A2	20070111	WO 2006-US26067	20060630
WO 2007005887	A3	20070419		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-695949P P 20050701
OTHER SOURCE(S): CASREACT 146:142515; MARPAT 146:142515
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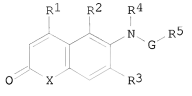
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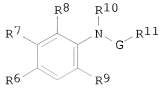
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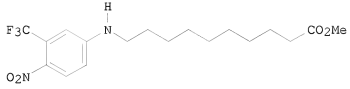
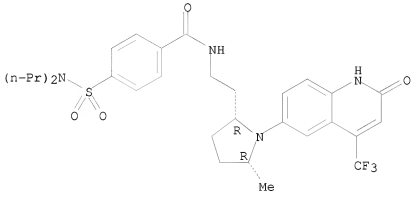

III

AB The invention relates to compds. of general formulas I, II or related derivs., which are androgen receptor modulators. In compds. I, X is O, S, or (un)substituted N; G is a bond, C(O), C(S), or S(O)2; R1, R2, and R3 are independently selected from H, halo, OH, SH, NH2, C1-6 alkoxy, C1-6 haloalkoxy, C1-6 alkylthio, C1-6 alkylamino, (un)substituted C1-4 alkyl, (un)substituted C1-4 haloalkyl, etc.; and R4 and R5 are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, etc.; including pharmaceutically acceptable salts and prodrugs thereof. In compds. II, G is as defined previously; R6 and R7 are independently selected from halo, cyano, nitro, C1-4 alkyl, C1-4 haloalkyl, C1-4 heteroalkyl, and C1-4 heterohaloalkyl; R8 and R9 are independently selected from H, halo, OH, SH, NH2, C1-6 alkoxy, C1-6 haloalkoxy, C1-6 alkylthio, C1-6 alkylamino, (un)substituted C1-4 alkyl, (un)substituted C1-4 haloalkyl, (un)substituted C1-4 heteroalkyl, etc.; and R10 and R11 are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, etc.; including pharmaceutically acceptable salts and prodrugs thereof. The invention also relates to the preparation of the compds. of the invention, pharmaceutical compns. comprising a compound of the invention and a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment or prevention of conditions that respond to androgen receptor modulation, such as acne, male-pattern baldness, infertility, and impotence. Substitution of Me 10-bromodecanoate with 4-nitro-3-trifluoromethylaniline gave aminodecanoate III. Some compds. of the invention are agonists of androgen receptors, but other compds. are antagonists of androgen receptors (no data).

IT 918895-56-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of quinolinones, chromenones,

benzothiopyranones, and anilines for use as androgen receptor modulators)
RN 918895-56-4 CA
CN Benzamide, N-[2-[(2R,5R)-1-[1,2-dihydro-2-oxo-4-(trifluoromethyl)-6-quinolinyl]-5-methyl-2-pyrrolidinyl]ethyl]-4-[(dipropylamino)sulfonyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 142:280067 CA
TITLE: Preparation of 6-pyrrolidinyl- and 6-piperidinylquinolinones as androgen receptor modulators
INVENTOR(S): Zhi, Lin; Martinborough, Esther; Shen, Yixing; Stevens Lau, Thomas Lot; Wu, Min; Long, Yun Oliver
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005018573	A2	20050303	WO 2004-US27483	20040823
WO 2005018573	A3	20050506		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,

	SN, TD, TG				
AU 2004266160		A1	20050303	AU 2004-266160	20040823
CA 2536349		A1	20050303	CA 2004-2536349	20040823
EP 1656142		A2	20060517	EP 2004-782052	20040823
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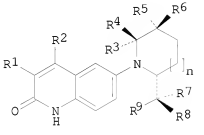
CN 1838956		A	20060927	CN 2004-80024125	20040823
BR 2004013820		A	20061024	BR 2004-13820	20040823
JP 2007503398		T	20070222	JP 2006-524121	20040823
MX 2006001751		A	20060512	MX 2006-1751	20060214
IN 2006MN00272		A	20070608	IN 2006-MN272	20060308
US 20070066650		A1	20070322	US 2006-566569	20060821
US 20080227810		A9	20080918		
IN 2009MN00090		A	20090515	IN 2009-MN90	20090109
PRIORITY APPLN. INFO.:				US 2003-497125P	P 20030822
				WO 2004-US27483	W 20040823
				IN 2006-MN272	A3 20060308

OTHER SOURCE(S): MARPAT 142:280067

GI



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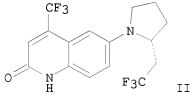


II

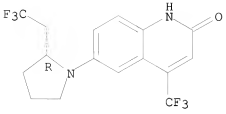
AB Title compds. I [wherein R1 = H, F, Cl or alkyl; R2 = H, halo, (un)substituted alkyl; R3, R4 = H, (un)substituted alkyl or (hetero)aryl; R5, R6 = OH, OPh, OBn or alkoxy; R5 - R8 = H, F, Cl or (un)substituted alkyl; R7 and R8 taken together form a CO; R9 = H, thioether, (un)substituted amine, alkyl, etc.; n = 0-1; and pharmaceutically acceptable salts thereof], e.g., II, were prepared as androgen receptor (AP) modulators. Biol. assays were performed, but no data were reported. Also disclosed are pharmaceutical compns. of I, methods for modulating processes mediated by AR, and their medical uses in the treatment of such as acne and sexual dysfunction.

IT 847235-72-7P, (R)-6-[2-(2,2,2-Trifluoroethyl)-1-pyrrolidinyl]-4-trifluoromethyl-2(1H)-quinolinone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(modulator; preparation of pyrrolidinyl- and piperidinylquinolinones as androgen receptor modulators)

RN 847235-72-7 CA

CN 2(1H)-Quinolinone, 6-[(2R)-2-(2,2,2-trifluoroethyl)-1-pyrrolidinyl]-4-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 5 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 134:207727 CA
TITLE: Preparation of quinolinones and related bicyclic compounds as androgen and progesterone receptor modulators.
INVENTOR(S): Zhi, Lin; Tegley, Christopher; Pio, Barbara; Arjan van Oeveren, Cornelis; Motamedi, Mehrnouch; Martinborough, Esther; West, Sarah; Higuchi, Robert; Hamann, Lawrence; Farmer, Luc
PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 356 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016108	A2	20010308	WO 2000-US23585	20000825
WO 2001016108	A3	20011220		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6566372	B1	20030520	US 2000-649466	20000824
CA 2384435	A1	20010308	CA 2000-2384435	20000825
BR 2000013653	A	20020514	BR 2000-13653	20000825
EP 1212303	A2	20020612	EP 2000-959507	20000825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200508	T2	20020923	TR 2002-508	20000825
CN 1382124	A	20021127	CN 2000-814750	20000825
CN 1262540	C	20060705		
JP 2003508387	T	20030304	JP 2001-519677	20000825
HU 2002004337	A2	20030328	HU 2002-4337	20000825
HU 2002004337	A3	20030630		
AU 782647	B2	20050818	AU 2000-70819	20000825

CN 1775759	A	20060524	CN 2005-10112855		20000825
CN 100384823	C	20080430			
CN 101029042	A	20070905	CN 2006-10078531		20000825
ZA 2002001053	A	20030528	ZA 2002-1053		20020206
IN 2002MN00201	A	20051104	IN 2002-MN201		20020215
NO 2002000912	A	20020429	NO 2002-912		20020225
MX 2002002027	A	20030519	MX 2002-2027		20020226
BG 106539	A	20021031	BG 2002-106539		20020321
US 20030130505	A1	20030710	US 2002-299909		20021118
US 6964973	B2	20051115			
US 20050288350	A1	20051229	US 2005-165769		20050623
PRIORITY APPLN. INFO.:			US 1999-150987P	P	19990827
			US 2000-649466	A3	20000824
			CN 2000-814750	A3	20000825
			WO 2000-US23585	W	20000825
			US 2002-299909	A3	20021118

OTHER SOURCE(S): MARPAT 134:207727

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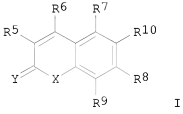


I

AB Title compds., e.g. [I; R1, R2 = COR3, CSR3, SO2R3, NO, NR3R4, alkyl, alkenyl, haloalkyl, haloalkenyl, haloalkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, etc.; R1R2 = atoms to form (substituted) heterocyclyl; R3, R4 = H, (substituted) alkyl, alkenyl, alkynyl, haloalkyl, heteroalkyl, heteroaryl, aryl; R5 = H, F, Cl, Br, iodo, OR3, SR3, NR3R4, alkyl, haloalkyl, heteroalkyl; R6 = F, Cl, Br, iodo, Me, CF3, CHF2, cyano, CF2Cl, CF2OR3, OR3, SOR3, CO2R3, NR3R4, (substituted) alkyl, alkenyl, alkynyl, haloalkyl, heteroalkyl, etc.; R7, R8 = H, F, Cl, Br, iodo, cyano, OR3, NR3R4, SR3, SOR3, NR3COR4, alkyl, haloalkyl, heteroalkyl, etc.; R9 = H, F, Cl, iodo, OR3, NR3R4, SR3, SOR3, SO2R3, alkyl, haloalkyl, heteroalkyl; R10 = NR1R2, (substituted) heterocyclyl; Y = O, S, NR3, NOR3, CR3R4], were prepared Thus, 6-amino-4-trifluoromethyl-2(1H)-quinolinone (preparation given) was stirred with propionaldehyde and NaBH3CN in MeOH to give 70-95% 6-propylamino-4-trifluoromethyl-2(1H)-quinolinone. The latter showed androgen receptor agonist activity with a potency of 27 nM. A drug composition is given. [This abstract record is one of 2 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 328949-98-0P

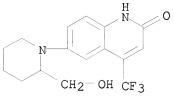
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

RN 328949-98-0 CA

CN 2(1H)-Quinolinone, 6-[2-(hydroxymethyl)-1-piperidinyl]-4-(trifluoromethyl)-

(CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'REGISTRY' ENTERED AT 13:22:05 ON 22 JUL 2009
L1 STRUCTURE UPLOADED
L2 9 S L1 SAM
L3 192 S L1 FULL

FILE 'CA' ENTERED AT 13:22:31 ON 22 JUL 2009
L4 5 S L3

FILE 'REGISTRY' ENTERED AT 13:23:46 ON 22 JUL 2009
L5 STRUCTURE UPLOADED
L6 173 S L5 FULL

FILE 'CA' ENTERED AT 13:24:39 ON 22 JUL 2009
L7 5 S L6

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Executing the logoff script...

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STN INTERNATIONAL LOGOFF AT 13:25:28 ON 22 JUL 2009